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Hilbert and Hadamard transforms by generalized Chebyshev expansion

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Abstract

An automatic quadrature is presented for approximating Hadamard finite-part (fp) integrals of a smooth function, with a double pole singularity within the range of integration. The quadrature rule is derived from the differentiation of an approximation to a Cauchy principal value integral or the Hilbert transform. The approximation to the fp integral is represented as a function of the value of pole by using Chebyshev polynomials of the second kind. Since the error can be estimated independently of the value of pole, a set of integrals for a set of values of pole can be efficiently approximated to a required tolerance, with the same number of function evaluations. Numerical examples are also included to illustrate the performance of the methods.

Key words: Hadamard finite-part integrals; Integral transform; Automatic quadrature; Singular integral; Hilbert transform; Cauchy principal value integrals; Chebyshev polynomial; FFT

1. Introduction

We present an automatic quadrature for approximating Hadamard finite-part (fp) integrals of the form

$$I(f;c) \equiv \fint_{-1}^{1} \frac{f(t)}{(t-c)^2}\,\mathrm{d}t = \frac{\mathrm{d}}{\mathrm{d}c} \fint_{-1}^{1} \frac{f(t)}{t-c}\,\mathrm{d}t, \quad -1 < c < 1, \tag{1}$$

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where $f(t)$ is assumed to be a smooth function on $[-1, 1]$ and the integral on the right is the Cauchy principal value (pv) integral or the Hilbert transform over a finite interval [4, p.11], [8]. There seems to be little literature on the automatic quadrature for fp integrals (1), although several papers [2,14–17] concern the numerical integration of fp integrals.

Although fp integrals may be defined in a few different, but equivalent, ways [15,16], the use of the definition in the right of (1) is helpful in deriving a quadrature rule for fp integrals. In fact, some authors apply their quadrature rules for principal value (pv) integrals to the relation (1) for obtaining the quadrature rule for fp integrals. Paget [17] utilizes the integration formula [6] for pv integrals to get a Gauss-type rule for fp integrals. Bialecki [2] adapts a Sinc quadrature rule [1] for pv integrals to derive the quadrature rule for fp integrals.

In either case of the quadrature rules, however, a numerical instability problem could arise because of the small number occurring in the denominator of the quadrature rules, when a sample point happens to be very close to the double pole c, see [2, (3.5)] [17, (2.9)]. This instability requires special care in programming the rules for computers.

The aim of the paper is to develop a numerically stable integration rule for fp integrals, and consequently we construct an efficient automatic quadrature of nonadaptive type for the Hadamard transform $I(f; c)$ (1) as a function of c under the assumption that the derivative $f'(t)$ is available. Our method also makes use of the definition on the right of (1) along with a quadrature rule [10] having no instability problem, based on the Chebyshev series expansion of $f(t)$ for pv integrals. Further, the sequence of Chebyshev approximations to $f(t)$ is recursively and efficiently generated by using the FFT [12] until a satisfactory approximation is obtained.

In Section 2 we briefly review a quadrature rule for pv integrals [10] and give a new expression of the approximation to the Hilbert transform as a function of c in terms of the Chebyshev polynomial of the first kind, see (9) below. From this expression, we show that an approximation to the Hadamard transform (1) as a function of c is represented by using the Chebyshev polynomial of the second kind, and by using a derivative $f'(c)$ as well as $f(c)$ at c, see (11) below.

In Section 3 we discuss the estimate of truncation error for the approximation to fp integrals. By assuming that $f(t)$ is analytic in an ellipse in the complex plane, it is found that the error can be bounded independently of the value of c on $(-1, 1)$. This fact enables us to construct an efficient automatic quadrature for evaluating, to a given absolute tolerance, the Hadamard transform $I(f; c)$ (1) with c allowed varied. Further, it is shown that once the automatic quadrature scheme has yielded the approximations to fp integrals satisfying the tolerance, then approximations with a bit higher accuracies to the Hilbert transform can also be easily obtained.

Numerical examples for fp integrals are reported in Section 4.

2. Quadrature rule by Chebyshev expansion

2.1. Approximation to the Hilbert transform

We begin with a brief review of a quadrature rule for pv integrals [10] with a modification in the expression, which will be shown to be suited for deriving a quadrature rule for approximating the fp integrals (1).

Hasegawa and Torii [10] extended the Clenshaw–Curtis method [3] (henceforth abbreviated to CC method) to pv integrals. In the CC method, $f(t)$ is approximated by a sum of Chebyshev polynomials of the first kind $T_k(t)$:

$$p_N(t) = \sum_{k=0}^{N}{}'' a_k^N T_k(t), \quad -1 \leqslant t \leqslant 1, \tag{2}$$

interpolating $f(t)$ at the $N+1$ abscissae $\cos(\pi j/N)$, $0 \leqslant j \leqslant N$. In (2) the double prime denotes the summation where the first and last terms are halved. If $f(t)$ is a smooth function, the truncated Chebyshev series (2) converges rapidly as N increases.

By using the approximation $p_N(t)$ (2), their rule [10] for pv integrals can be written as follows:

$$\begin{aligned} ⨍_{-1}^{1} \frac{f(t)}{t-c}\,\mathrm{d}t &= \int_{-1}^{1} \frac{p_N(t)-p_N(c)}{t-c}\,\mathrm{d}t + f(c)\ln\left(\frac{1-c}{1+c}\right) + r_N(f;\,c) \\ &= 2\sum_{k=0}^{[(N-1)/2]}{}' \frac{d_{2k}(c)}{1-4k^2} + f(c)\ln\left(\frac{1-c}{1+c}\right) + r_N(f;\,c), \end{aligned} \tag{3}$$

where the $d_k(c)$'s are defined by the relation

$$p_N(t) - p_N(c) = (t-c)\sum_{k=0}^{N-1}{}' d_k(c) T_k(t), \tag{4}$$

and satisfy a three-term recurrence relation, see [10, (1.11)]. In (3), $r_N(f;\,c)$ is the remainder term and the prime denotes the summation whose first term is halved.

To incorporate the rule (3) into the quadrature rule for fp integrals, it is convenient to expand the first term of the right-hand side of (3) in terms of $T_k(c)$.

Lemma 2.1. *Let $p_N(t)$ be a polynomial of degree N defined by* (2). *Then we have*

$$\int_{-1}^{1} \frac{p_N(t)-p_N(c)}{t-c}\,\mathrm{d}t = 4\sum_{k=0}^{N-1}{}' A_k^N T_k(c), \quad -1 < c < 1, \tag{5}$$

where A_k^N is defined by

$$A_k^N = \sum_{n=0}^{[(N-k-1)/2]} \frac{a_{2n+k+1}^N}{2n+1}, \quad 1 \leqslant k \leqslant N-1, \tag{6}$$

and we take $\frac{1}{2}a_N^N$ instead of a_N^N.

Proof. Elliott [5] gives the identity involving Chebyshev polynomials of the second kind $U_k(t)$ defined by $U_k(t) = \sin\{(k+1)\theta\}/\sin\,\theta$, $t = \cos\,\theta$:

$$T_{n+1}(t) - T_{n+1}(c) = 2(t-c)\sum_{k=0}^{n}{}' U_{n-k}(t) T_k(c), \tag{7}$$

see also [10, (A.3)]. From (2) and (7) it follows that

$$\int_{-1}^{1} \frac{p_N(t)-p_N(c)}{t-c}\,\mathrm{d}t = 2\sum_{n=0}^{N-1} a_{n+1}^N \sum_{k=0}^{n}{}' T_k(c)\int_{-1}^{1} U_{n-k}(t)\,\mathrm{d}t, \tag{8}$$

where we take $\frac{1}{2}a_N^N$ instead of a_N^N. If one notes in (8) that the integral $\int_{-1}^{1} U_{n-1}(t)\, \mathrm{d}t$ equals $2/n$ if n is odd and vanishes otherwise, (5) follows easily. □

From (3) and (5) the quadrature rule for pv integrals can be rewritten in terms of the Chebyshev polynomial $T_k(c)$:

$$⨍_{-1}^{1} \frac{f(t)}{t-i}\, \mathrm{d}t = 4 \sum_{k=0}^{N-1}{}' A_k^N T_k(c) + f(c) \ln\left(\frac{1-c}{1+c}\right) + r_N(f;\, c). \tag{9}$$

This expression is also suited for deriving a rule for fp integrals.

2.2. Quadrature formula for the Hadamard transform

Now we present a numerically stable quadrature rule $Q_N(f;\, c)$ below for fp integrals (1). We will observe that the identity (5) enables us to represent the approximate integration as a function of c. Using (9) in (1) and noting that $\mathrm{d}T_k(c)/\mathrm{d}c = kU_{k-1}(c)$, we have

$$I(f;\, c) = Q_N(f;\, c) + R_N(f;\, c), \tag{10}$$

where a quadrature rule $Q_N(f;\, c)$ for fp integrals is given by

$$Q_N(f;\, c) = 4 \sum_{k=1}^{N-1} (kA_k^N) U_{k-1}(c) + f'(c) \ln\left(\frac{1-c}{1+c}\right) - \frac{2f(c)}{1-c^2}, \tag{11}$$

and $R_N(f;\, c)$ denotes the remainder term given by

$$R_N(f;\, c) = \frac{\mathrm{d}r_N(f;\, c)}{\mathrm{d}c}. \tag{12}$$

In (11) A_k^N is given by (6).

The sum in (11) can be efficiently evaluated with $N-2$ multiplications by Clenshaw's algorithm, for each value of c, provided $N-1$ products kA_k^N, $1 \leqslant k \leqslant N$, have been evaluated and stored in the memory of computer. On the other hand, the summations in (6) require $\frac{1}{4}(N-2)^2$ divisions for $1 \leqslant k < N$, although the amount of computation reduces to $O(N \log_2 N)$ if we resort to the convolution technique based on the FFT [13, p.57]. Consequently, to evaluate the first terms of the right-hand side of (11) to compute M approximations $Q_N(f;\, c)$'s for M values of c requires $O(MN + \frac{1}{4}N^2)$ multiplications (and divisions). Therefore, when we want to approximate the fp integrals for single or a very few values of c, it might be preferable to modify the expression in the first term of the right-hand side of (11) for efficiently computing the approximation $Q_N(f;\, c)$; we refer readers to Appendix A.

We remark that $Q_N(f;\, c)$ is a quadrature rule of noninterpolatory type because $Q_N(f;\, c)$ has degree of exactness $N-1$, using the function value $f(c)$ and the derivative $f'(c)$ at c, as well as N function evaluations for interpolating $f(t)$.

Incidentally, an automatic quadrature of nonadaptive type is generally constructed from the sequence of the approximations $\{Q_N\}$ converging to the integral $I(f;\, c)$, having an adequate method of error estimation, until a stopping criterion is satisfied. It is a usual and simple way to double the degree N of $p_N(t)$ (2) for generating the sequence $\{Q_N(f;\, c)\}$ (11). In order to make an automatic quadrature efficient, however, it is advantageous to have more changes of checking the stopping criterion than doubling N. In the following, we briefly review [12] that we can allow N to take the form 3×2^n and 5×2^n, as well as 2^n.

2.3. Generalized Chebyshev expansion

Here and henceforth we assume that N is a power of 2: 2^n, $n = 2, 3, \ldots$. Now, we will outline the iterative procedure [12] for computing the sequence of the truncated Chebyshev series, $\{p_N, p_{5N/4}, p_{3N/2}\}$, $N = 2^n$, $n = 2, 3, \ldots,$ until a stopping criterion described in Section 3 is satisfied.

Let $t_j^N = \cos(\pi j/N)$, $0 \leqslant j \leqslant N$, be the zeros of the polynomial $\omega_{N+1}(t)$ defined by

$$\omega_{N+1}(t) = T_{N+1}(t) - T_{N-1}(t) = 2(t^2 - 1)U_{N-1}(t). \tag{13}$$

Then, the coefficients a_k^N of $p_N(t)$ (2) are determined so that $p_N(t)$ interpolates $f(t)$ at the abscissae t_j^N, and consequently a_k^N is represented in the form

$$a_k^N = \frac{2}{N} \sum_{j=0}^{N}{}'' f\left(\cos\frac{\pi j}{N}\right) \cos\frac{\pi kj}{N}, \quad 0 \leqslant k \leqslant N. \tag{14}$$

The right-hand side of (14) is known to be efficiently computed by means of the FFT for real data [9].

For integer $\sigma = 2$ and 4, let $\{v_j^{N/\sigma}\}$, $0 \leqslant j < N/\sigma$, be a subset of the zeros of $T_N(t)$; in particular, be chosen to agree with a set consisting of the N/σ zeros of $T_{N/\sigma}(t) - \cos\{3\pi/(2\sigma)\}$. Then, we represent the polynomials $p_{N+N/\sigma}(t)$, $\sigma = 2, 4$, interpolating $f(t)$ at the nodes $v_j^{N/\sigma}$, $0 \leqslant j < N/\sigma$, $\sigma = 2, 4$, as well as at the zeros of $\omega_{N+1}(t)$ (13) in the Newton form:

$$\begin{aligned} p_{N+N/\sigma}(t) - p_N(t) &= -\omega_{N+1}(t) \sum_{k=1}^{N/\sigma} b_k^{N/\sigma} U_{k-1}(t) \\ &= \sum_{k=1}^{N/\sigma} b_k^{N/\sigma} \{T_{N-k}(t) - T_{N+k}(t)\}. \end{aligned} \tag{15}$$

The coefficients $\{b_k^{N/\sigma}\}$ are determined to satisfy the condition

$$f\left(v_j^{N/\sigma}\right) = p_{N+N/\sigma}\left(v_j^{N/\sigma}\right), \quad 0 \leqslant j < \frac{N}{\sigma}, \quad \sigma = 2, 4, \tag{16}$$

and the FFT [12] is used for efficiently evaluating the coefficients $b_k^{N/\sigma}$. We note that the set of $\frac{1}{4}N$ abscissae $\{v_j^{N/4}\}$, $0 \leqslant j < \frac{1}{4}N$, for $p_{5N/4}(t) - p_N(t)$ is contained in the $\frac{1}{2}N$ abscissae $\{v_j^{N/2}\}$, $0 \leqslant j < \frac{1}{2}N$, for $p_{3N/2}(t) - p_N(t)$, which is also included in the set of the N zeros of $T_N(t)$ $(= \omega_{2N+1}(t)/\{2\omega_{N+1}(t)\})$ for $p_{2N}(t) - p_N(t)$. This fact allows the iterative algorithm of computing the sequence $\{p_{3m}, p_{4m}, p_{5m}\}$, $m = 2^n$, $n = 1, 2, \ldots,$ using the FFT, see [12] for details.

3. Error estimate

Define $a_k^{N+N/\sigma}$, $\sigma = 2, 4$, by

$$a_k^{N+N/\sigma} = \begin{cases} a_k^N, & 0 \leqslant k < N - N/\sigma, \\ a_k^N + b_{N-k}^{N/\sigma}, & N - N/\sigma \leqslant k < N, \\ \frac{1}{2}a_N^N, & k = N, \\ -b_{k-N}^{N/\sigma}, & N < k \leqslant N + N/\sigma. \end{cases} \tag{17}$$

Then the quadrature rules $Q_{N+N/\sigma}(f;\ c)$, $\sigma=2, 4$, based on the polynomials $p_{N+N/\sigma}(t)$ (15) are given by the right-hand side of (11) with a_k^N replaced by $a_k^{N+N/\sigma}$ (17), where the outer sum ranges from 1 to $N+N/\sigma-1$ and the inner sum from 0 to $[\frac{1}{2}(N+N/\sigma-k-1]$.

Here, we will give error estimates for the approximations $Q_N(f;\ c)$, $Q_{5N/4}(f;\ c)$ and $Q_{3N/2}(f;\ c)$, especially for the analytic function f. Let ϵ_ρ denote the ellipse in the complex plane $z=x+\mathrm{i}y$ with foci $(x, y)=(-1, 0)$, $(1, 0)$ and semimajor axis $a=\frac{1}{2}(\rho+\rho^{-1})$ and semiminor axis $b=\frac{1}{2}(\rho-\rho^{-1})$ for a constant $\rho>1$.

Assume that $f(z)$ is single-valued and analytic inside and on ϵ_ρ. Then it follows from [10, (3.5) and (3.6)] that the remainder $r_N(f;\ c)$ of the approximation to pv integrals (3) can be expressed in the form

$$r_N(f;\ c)=\sum_{k=0}^{\infty}{}' \Omega_k^N(c)V_k^N(f), \tag{18}$$

where $\Omega_k^N(c)$ and $V_k^N(f)$ are defined by

$$\Omega_k^N(c)=\int_{-1}^{1}\frac{\omega_{N+1}(t)T_k(t)-\omega_{N+1}(c)T_k(c)}{t-c}\,\mathrm{d}t, \tag{19}$$

$$V_k^N(f)=\frac{1}{\pi^2\mathrm{i}}\oint_{\epsilon_\rho}\frac{\tilde{U}_k(z)f(z)\,\mathrm{d}z}{\omega_{N+1}(z)},\quad k\geqslant 0. \tag{20}$$

In (20), $\tilde{U}_k(z)$ is the Chebyshev function of the second kind defined by

$$\tilde{U}_k(z)=\int_{-1}^{1}\frac{T_k(t)\,\mathrm{d}t}{(z-t)\sqrt{1-t^2}}=\frac{\pi}{\sqrt{z^2-1}\,w^k}=\frac{2\pi}{(w-w^{-1})w^k}, \tag{21}$$

where $w=z+\sqrt{z^2-1}$ and $|w|>1$ for $z\notin[-1, 1]$ [7,11]. Similarly, from [10, Theorem 3.3], the remainder $r_{N+N/\sigma}(f;\ c)$ for the approximation, using $p_{N+N/\sigma}(t)$, to pv integrals might be written as follows:

$$r_{N+N/\sigma}(f;\ c)=\frac{1}{2}\sum_{k=0}^{\infty}{}'\left\{\Omega_k^{N+N/\sigma}(c)+\Omega_k^{N-N/\sigma}(c)-2\Omega_k^N(c)\cos\frac{3\pi}{2\sigma}\right\}V_k^{N+N/\sigma}(f),$$
$$\sigma=2, 4, \tag{22}$$

where $V_k^{N+N/\sigma}(f)$ is defined by

$$V_k^{N+N/\sigma}(f)=\frac{1}{\pi^2\mathrm{i}}\oint_{\epsilon_\rho}\frac{\tilde{U}_k(z)f(z)\,\mathrm{d}z}{\omega_{N+1}(z)\{T_{N/\sigma}(z)-\cos\{3\pi/(2\sigma)\}\}},\quad k\geqslant 0,\quad \sigma=2, 4. \tag{23}$$

Now we proceed to estimate the remainder $R_N(f;\ c)$ of the quadrature rule $Q_N(f;\ c)$ (11) for fp integrals (1). From (10), (12) and (18) the remainder $R_N(f;\ c)$ can be written as follows:

$$I(f;\ c)-Q_N(f;\ c)\equiv R_N(f;\ c)=\sum_{k=0}^{\infty}{}'\frac{\mathrm{d}\Omega_k^N(c)}{\mathrm{d}c}V_k^N(f). \tag{24}$$

The estimation (24) of $R_N(f;\ c)$ requires a bound for $\mathrm{d}\Omega_k(c)/\mathrm{d}c$ as well as one for $V_k^N(f)$. To this end, it is convenient to express $\Omega_k^N(c)$ using a polynomial $S_m(x)$ defined as follows.

Definition 3.1. For integer $m \geqslant 1$, a polynomial $S_m(x)$ of degree m is defined by

$$S_m(x) = \sum_{n=0}^{m}{}'' T_{m-n}(x) \int_{-1}^{1} T_n(t)\, \mathrm{d}t, \quad m = 1, 2, \dots . \tag{25}$$

Further, we define $S_{-m}(x) = -S_m(x)$ and $S_0(x) = 0$.

Using (19) and [10, (A.4)] gives the following lemma.

Lemma 3.2. *For $\Omega_k^N(c)$ defined by* (19), *we have*

$$\tfrac{1}{2}\Omega_k^N(c) = S_{N+k}(c) + S_{N-k}(c), \tag{26}$$

where $S_m(x)$ is defined by Definition 3.1.

Appendix B proves the following lemma.

Lemma 3.3. *For integer $n \geqslant 3$ define $G(n)$ by*

$$G(n) = n \ln(n-2) + n + 2 + \frac{2}{n-1}, \quad n = 3, 4, \dots . \tag{27}$$

Further we define $G(1) = \frac{1}{2}$ and $G(2) = 2$. Then, for $S_m(x)$ defined by (25), $\mathrm{d}S_m(x)/\mathrm{d}x$ *is bounded independently of x by*

$$\left| \frac{\mathrm{d}S_m(x)}{\mathrm{d}x} \right| \leqslant 2G(m), \quad m = 1, 2, \dots . \tag{28}$$

From (24), (26) and (28) we have the following theorem.

Theorem 3.4. *Let $N = 2^n$, $n = 2, 3, \dots$, and assume that $f(z)$ is single-valued analytic inside and on ϵ_p. Then, the error of the approximation $Q_N(f;\, c)$* (11) *to the fp integrals* (1) *is bounded independently of c by*

$$\begin{aligned} &|I(f;\, c) - Q_N(f;\, c)| \\ &\quad \leqslant 4\left\{ \sum_{k=N}^{\infty} G(k)\left|V_{k-N}^N(f)\right| + \sum_{k=1}^{N-1} G(k)\left|V_{N-k}^N(f)\right| + \sum_{k=1}^{\infty} G(k)\left|V_{k+N}^N(f)\right| \right\}, \end{aligned} \tag{29}$$

where $V_k^N(f)$ and $G(k)$ are given by (20) *and* (27), *respectively.*

Suppose that $f(z)$ is a meromorphic function which has M simple poles at the points z_m, $m = 1, 2, \dots, M$, outside ϵ_p with residues Res $f(z_m)$. Then, performing the contour integral of (20) yields

$$V_k^N(f) = -\frac{2}{\pi} \sum_{m=1}^{M} \operatorname{Res} f(z_m) \frac{\tilde{U}_k(z_m)}{\omega_{N+1}(z_m)}, \quad k \geqslant 0. \tag{30}$$

Defining $r = \min_{1 \leqslant m \leqslant M} | z_m + \sqrt{z_m^2 - 1} | > 1$, we can see from (21) and (30) that $\rho < r$ and $| V_k^N(f) | \simeq | V_0^N(f) | r^{-k} = \mathrm{O}(r^{-k-N})$. This fact and (29) allow the estimation of the error:

$$\begin{aligned} | I(f; c) - Q_N(f; c) | &\lesssim 4 \left| V_0^N(f) \right| \left\{ \sum_{k=N}^{\infty} G(k) r^{N-k} + \sum_{k=1}^{N-1} G(k) r^{k-N} + \sum_{k=1}^{\infty} G(k) r^{-k-N} \right\} \\ &= 4 \left| V_0^N(f) \right| \frac{r+1}{r-1} \left[N(\ln N + 1) \left\{ 1 + \mathrm{O}\left(\frac{1}{N} \right) \right\} + \mathrm{O}(r^{-N}) \right]. \end{aligned} \tag{31}$$

Next, we wish to estimate $| V_0^N(f) |$ in terms of the available coefficients a_k^N of $p_N(t)$. Elliott [5] gives

$$a_k^N = \frac{2}{\pi \mathrm{i}} \oint_{\epsilon_p} \frac{T_{N-k}(z) f(z)}{\omega_{N+1}(z)} \, \mathrm{d}z, \quad 0 \leqslant k \leqslant N.$$

Performing the contour integral and comparing the result with (30) yields the estimates

$$\left| V_0^N(f) \right| \sim \frac{| a_N^N | r}{r^2 - 1}, \tag{32}$$

and $| a_k^N | \sim r | a_{k+1}^n |$, unless the poles z_m are close to the segment $[-1, 1]$ on the real axis. Finally, from (31) and (32) we could obtain an estimate of the truncation error for $Q_N(f; c)$ as follows:

$$E_N(f; c) = 8\left(\tfrac{1}{2} | a_N^N | \right) N(\ln N + 1) \frac{r}{(r-1)^2} \quad (\rightarrow 0, \quad \text{if } N \rightarrow \infty), \tag{33}$$

where we note that $\frac{1}{2} a_N^N$ are the coefficients of the last term in the truncated Chebyshev series (2). The constant r may be estimated from the asymptotic behavior of $\{a_k^N\}$ [12].

Similarly, comparing (22), (24) and (31) suggests the estimation of the remainder $R_{N+N/\sigma}(f; c)$ of the approximation $Q_{N+N/\sigma}(f; c)$ based on $p_{N+N/\sigma}(t)$ to fp integrals:

$$\begin{aligned} &\left| I(f; c) - Q_{N+N/\sigma}(f; c) \right| \\ &\quad \equiv \left| \frac{\mathrm{d} r_{N+N/\sigma}(f; c)}{\mathrm{d}c} \right| \\ &\quad \lesssim 2 \left| V_0^{N+N/\sigma}(f) \right| \frac{r+1}{r-1} \left[\left\{ L_N\left(\frac{1}{\sigma} \right) + L_N(0) \left| \cos \frac{3\pi}{2\sigma} \right| \right\} \left\{ 1 + \mathrm{O}\left(\frac{1}{N} \right) \right\} + \mathrm{O}(r^{-N}) \right] \\ &\quad \sim 2 \left| V_0^{N+N/\sigma}(f) \right| \frac{r+1}{r-1} \left[\left\{ 1 + \left| \cos \frac{3\pi}{2\sigma} \right| \right\} L_N(0) + Nl\left(\frac{1}{\sigma} \right) \right], \quad \sigma = 2, 4, \end{aligned} \tag{34}$$

where we define $l(x)$ and $L_N(x)$ for $0 \leqslant x < 1$, respectively, by

$$l(x) = (1 + x) \ln(1 + x) + (1 - x) \ln(1 - x), \tag{35}$$

$$L_N(x) = (N + Nx)\{\ln(N + Nx) + 1\} + (N - Nx)\{\ln(N - Nx) + 1\}. \tag{36}$$

From [10, (3.22)], we see that $|V_0^{N+N/\sigma}| \sim 4|b_{N/\sigma}^{N/\sigma}|r/(r^2-1)$, $|V_k^{N+N/\sigma}| = \mathrm{O}(r^{-k-N-N/\sigma})$ and $|b_k^{N/\sigma}| \sim r|b_{k+1}^{N/\sigma}|$. Using these relations in (34), one gets estimates of the truncation errors $E_{N+N/\sigma}(f;\, c)$ for the approximations $Q_{N+N/\sigma}(f;\, c)$, $\sigma = 2, 4$, as follows:

$$E_{N+N/\sigma}(f;\, c) = 8\left|b_{N/\sigma}^{N/\sigma}\right|\left[2\left\{1+\left|\cos\frac{3\pi}{2\sigma}\right|\right\}(\ln\, N+1) + l\left(\frac{1}{\sigma}\right)\right]N\frac{r}{(r-1)^2}$$
$$\to 0 \quad (\text{if } N\to\infty), \quad \sigma = 2, 4. \tag{37}$$

It should be noted that the error estimates (33) and (37) for the quadrature rules $Q_N(f;\, c)$ and $Q_{N+N/\sigma}(f;\, c)$, respectively, are independent of the value of c. This indicates that the approximate polynomials $p_N(t)$, $p_{5N/4}(t)$ or $p_{3N/2}(t)$ can be used common to the set of the integrals $I(f;\, c)$ for a set of c-values if a stopping criterion (33) or (37) is satisfied.

Furthermore, we remark that the polynomials $p_N(t)$, $p_{5N/4}(t)$ or $p_{3N/2}(t)$ can be used commonly, not only for the Hadamard transform, but also for the Hilbert transform. To see this, let $E_N^{(\mathrm{pv})}(f;\, c)$ and $E_{N+N/\sigma}^{(\mathrm{pv})}(f;\, c)$ denote the estimates of the truncation errors for the approximations to pv integrals. Then, from [10, (3.19), (3.23) and (3.24)] and from (33) and (37) it follows that

$$\frac{E_N(f;\, c)}{E_N^{(\mathrm{pv})}(f;\, c)} = N\{\ln\, N+1\},$$

$$\frac{E_{N+N/\sigma}(f;\, c)}{E_{N+N/\sigma}^{(\mathrm{pv})}(f;\, c)} = N\left\{\ln\, N+1+\frac{l(1/\sigma)}{2[1+|\cos\{3\pi/(2\sigma)\}|]}\right\}, \quad \sigma = 2, 4.$$

These ratios suggest that the accuracy of an approximation obtained by using the quadrature rule (9) for pv integrals is higher than that of the approximation (11) for fp integrals, using the same number of function evaluations. Consequently, once an approximation to fp integrals, satisfying the stopping criterion (33) or (37), has been obtained, an approximation to pv integrals having a bit higher accuracy can be easily computed only by applying the Clenshaw's algorithm to the summation in (9).

4. Numerical examples

In this section we illustrate the performance of the present automatic quadrature scheme for the following integrals having a parameter a:

(A) $$I_1(a,\, c) = \displaystyle\neq\!\!\!\!\!\!\int_{-1}^{1} \frac{(a^2-t^2)^{-1/2}}{(t-c)^2}\,\mathrm{d}t, \quad a = 1.1,\, 1.01,\, 1.005,$$

(B) $$I_2(a,\, c) = \displaystyle\neq\!\!\!\!\!\!\int_{-1}^{1} \frac{\mathrm{e}^{a(t-1)}}{(t-c)^2}\,\mathrm{d}t, \quad a = 4,\, 8,\, 16,$$

(C) $$I_3(a, c) = \fint_{-1}^{1} \frac{(t^2+a^2)^{-1}}{(t-c)^2} \, \mathrm{d}t, \quad a = 1, \tfrac{1}{4}, \tfrac{1}{8},$$

(D) $$I_4(a, c) = \fint_{0}^{1} \frac{\cos(2\pi a t)}{(t-c)^2} \, \mathrm{d}t, \quad a = 8, 16, 32,$$

(E) $$I_5(a, c) = \fint_{-1}^{1} \frac{1-a^2}{1-2at+a^2} \frac{1}{(t-c)^2} \, \mathrm{d}t, \quad a = 0.7, 0.8, 0.9.$$

Paget [17] uses (A) for testing his integration rule. The integrals I_1 [17], I_3 and I_5 are analytically integrated, respectively, as follows:

$$I_1(a, c) = \frac{c}{d^3} \ln\left(\frac{d-cg}{d+cg}\right) - \frac{2g}{d(1-c^2)^{1/2}}, \quad \text{where } d = (a^2-c^2)^{1/2}, \; g = (a^2-1)^{1/2},$$

$$I_3(a, c) = \frac{2c}{(a^2+c^2)^2} \left\{ \frac{2c}{a} \tan^{-1}\frac{1}{a} - \ln\left(\frac{1-c}{1+c}\right) \right\} - \frac{2}{a^2+c^2} \left\{ \frac{1}{1-c^2} + \frac{1}{a} \tan^{-1}\frac{1}{a} \right\},$$

$$I_5(a, c) = \frac{2a(1-a^2)}{(1-2ca+a^2)^2} \left\{ \ln\left(\frac{1-c}{1+c}\right) - 2\ln\left(\frac{1-a}{1+a}\right) \right\} - \frac{2(1-a^2)}{(1-2ca+a^2)(1-c^2)}.$$

In Table 1 we show the numbers of function evaluations, required to achieve the requested accuracies, $\epsilon_a = 10^{-6}$ and 10^{-10}, and the actual and estimated errors, for the integrals (A)–(E). The errors are estimated by using (33) or (37), where for simplicity we have replaced the factor $r/(r-1)^2$ by unity, assuming that the truncated Chebyshev series (2) and (15) converge rapidly, i.e., r is greater than and not close to unity. Table 2 lists the actual errors as well as the estimated errors, obtained by using the present automatic quadrature scheme to approximate the integral (A) for a variety of c-values to the required tolerances of $\epsilon_a = 10^{-4}$, 10^{-7} and 10^{-10}.

It should be noted that the present method can efficiently give all the approximations to the integrals for a set of c-values by using the common number of function evaluations once and for all, except for the evaluations of each function value $f(c)$ and derivative $f'(c)$ at c, for a smooth function $f(t)$.

The computation was carried out in double-precision arithmetic (about sixteen significant digits).

The FORTRAN program implementing the present method will appear elsewhere, but presently is available from the first author.

Appendix A

It may be preferable to modify the expression in the first term of the right-hand side of (11), if we like to approximate the fp integrals (1) for single or a very few c-values.

Table 1
Performance of the present method for the integrals $⨍_{-1}^{1} f(t)/(t-c)^2\, dt$, where (A) $f(t)=(a^2-t^2)^{-1/2}$; (B) $f(t)=e^{a(t-1)}$; (C) $f(t)=(t^2+a^2)^{-1}$; (D) $f(t)=\cos(2\pi at)$; (E) $f(t)=(1-a^2)/(1-2at+a^2)$

$f(t)$	a	$\epsilon_a=10^{-6}$				$\epsilon_a=10^{-10}$			
		N	Error			N	Error		
			$c=0.35$	0.95	Estimate		$c=0.35$	0.95	Estimate
(A)	1.1	$65_{+1+(1)}$	$5\cdot10^{-12}$	$9\cdot10^{-11}$	$7\cdot10^{-10}$	$81_{+1+(1)}$	$8\cdot10^{-15}$	$4\cdot10^{-13}$	$1\cdot10^{-12}$
	1.01	$161_{+1+(1)}$	$8\cdot10^{-10}$	$4\cdot10^{-7}$	$1\cdot10^{-6}$	$257_{+1+(1)}$	$2\cdot10^{-14}$	$2\cdot10^{-12}$	$2\cdot10^{-11}$
	1.005	$257_{+1+(1)}$	$2\cdot10^{-10}$	$1\cdot10^{-8}$	$7\cdot10^{-8}$	$385_{+1+(1)}$	$2\cdot10^{-13}$	$1\cdot10^{-11}$	$4\cdot10^{-11}$
(B)	4	$17_{+1+(1)}$	$1\cdot10^{-9}$	$1\cdot10^{-9}$	$6\cdot10^{-7}$	$25_{+1+(1)}$	$3\cdot10^{-14}$	$2\cdot10^{-12}$	$5\cdot10^{-13}$
	8	$25_{+1+(1)}$	$6\cdot10^{-12}$	$2\cdot10^{-11}$	$1\cdot10^{-8}$	$33_{+1+(1)}$	$4\cdot10^{-14}$	$6\cdot10^{-12}$	$7\cdot10^{-14}$
	16	$33_{+1+(1)}$	$2\cdot10^{-11}$	$4\cdot10^{-11}$	$2\cdot10^{-9}$	$41_{+1+(1)}$	$4\cdot10^{-14}$	$1\cdot10^{-11}$	$1\cdot10^{-12}$
(C)	1	$33_{+1+(1)}$	$3\cdot10^{-11}$	$6\cdot10^{-11}$	$2\cdot10^{-9}$	$41_{+1+(1)}$	$9\cdot10^{-14}$	$2\cdot10^{-13}$	$3\cdot10^{-12}$
	$\frac{1}{4}$	$129_{+1+(1)}$	$1\cdot10^{-10}$	$5\cdot10^{-11}$	$2\cdot10^{-9}$	$161_{+1+(1)}$	$5\cdot10^{-13}$	$3\cdot10^{-12}$	$1\cdot10^{-12}$
	$\frac{1}{8}$	$257_{+1+(1)}$	$1\cdot10^{-10}$	$1\cdot10^{-10}$	$6\cdot10^{-9}$	$321_{+1+(1)}$	$3\cdot10^{-12}$	$1\cdot10^{-11}$	$6\cdot10^{-12}$
(D)	8	$81_{+1+(1)}$	$1\cdot10^{-9}$	$3\cdot10^{-9}$	$7\cdot10^{-7}$	$97_{+1+(1)}$	$4\cdot10^{-12}$	$4\cdot10^{-11}$	$4\cdot10^{-12}$
	16	$161_{+1+(1)}$	$8\cdot10^{-12}$	$1\cdot10^{-10}$	$6\cdot10^{-12}$	$161_{+1+(1)}$	$8\cdot10^{-12}$	$1\cdot10^{-10}$	$6\cdot10^{-12}$
	32	$257_{+1+(1)}$	$3\cdot10^{-11}$	$8\cdot10^{-11}$	$4\cdot10^{-9}$	$321_{+1+(1)}$	$2\cdot10^{-11}$	$7\cdot10^{-12}$	$3\cdot10^{-11}$
(E)	0.7	$81_{+1+(1)}$	$8\cdot10^{-11}$	$6\cdot10^{-10}$	$2\cdot10^{-8}$	$97_{+1+(1)}$	$6\cdot10^{-13}$	$3\cdot10^{-12}$	$9\cdot10^{-11}$
	0.8	$129_{+1+(1)}$	$5\cdot10^{-10}$	$4\cdot10^{-9}$	$1\cdot10^{-8}$	$161_{+1+(1)}$	$3\cdot10^{-13}$	$4\cdot10^{-11}$	$5\cdot10^{-11}$
	0.9	$257_{+1+(1)}$	$1\cdot10^{-9}$	$4\cdot10^{-8}$	$1\cdot10^{-7}$	$1025_{+1+(1)}$	$5\cdot10^{-12}$	$1\cdot10^{-10}$	$1\cdot10^{-10}$

The numbers N of function evaluations required to satisfy the requested tolerances $\epsilon_a=10^{-6}$ and 10^{-10} are listed in the third and seventh columns, where the unities inside and outside of the parentheses denote the numbers of evaluation of the derivative $f'(c)$ and the function value $f(c)$, respectively, for each value of c.

Table 2
Actual errors and estimated errors, obtained by using the present method for the integral $⨍_{-1}^{1}(a^2-t^2)^{-1/2}/(t-c)^2\, dt$ with $a=1.01$ kept fixed and with c allowed varied

c	Integral	$\epsilon_a=10^{-4}$	$\epsilon_a=10^{-7}$	$\epsilon_a=10^{-10}$
0.09	−0.284 717 463 933 291 3	$1.7\cdot10^{-7}$	$5.6\cdot10^{-11}$	$3.2\cdot10^{-13}$
0.19	−0.309 525 948 295 357 3	$3.0\cdot10^{-7}$	$1.0\cdot10^{-10}$	$1.3\cdot10^{-13}$
0.29	−0.357 988 660 619 348 9	$1.6\cdot10^{-7}$	$5.6\cdot10^{-11}$	$8.9\cdot10^{-14}$
0.39	−0.442 578 385 003 418 8	$6.4\cdot10^{-7}$	$2.3\cdot10^{-10}$	$5.7\cdot10^{-14}$
0.49	−0.590 516 238 229 471 9	$9.6\cdot10^{-7}$	$7.6\cdot10^{-11}$	$3.1\cdot10^{-13}$
0.59	−0.866 593 353 426 147 1	$1.9\cdot10^{-6}$	$9.3\cdot10^{-11}$	$4.1\cdot10^{-13}$
0.69	−1.453 778 199 318 205	$1.2\cdot10^{-6}$	$4.5\cdot10^{-10}$	$5.0\cdot10^{-13}$
0.79	−3.045 471 141 426 866	$1.3\cdot10^{-6}$	$3.2\cdot10^{-10}$	$9.4\cdot10^{-13}$
0.89	−10.407 440 276 871 14	$1.1\cdot10^{-5}$	$2.5\cdot10^{-9}$	$2.5\cdot10^{-12}$
0.99	−571.741 847 189 376 0	$3.0\cdot10^{-5}$	$1.9\cdot10^{-9}$	$6.9\cdot10^{-12}$
Estimated error		$6.3\cdot10^{-5}$	$1.7\cdot10^{-8}$	$1.8\cdot10^{-11}$
$N-1-(1)$		129	193	257

The numbers N of function evaluations in the last row, required to satisfy absolute tolerances $\epsilon_a=10^{-4}$, 10^{-7} and 10^{-10}, are the same for all integrals with the c-values listed, except for the evaluations of function values $f(c)$ and derivatives $f'(c)$.

One can also rewrite (8) as follows:

$$\int_{-1}^{1} \frac{p_N(t)-p_N(c)}{t-c}\,\mathrm{d}t = 2\sum_{n=0}^{[(N-1)/2]} \frac{u_{2n}(c)}{2n+1}, \tag{38}$$

where $u_n(c)$ is defined by

$$u_n(c) = 2\sum_{m=n}^{N-1}{}' a_{m+1}^N T_{m-n}(c), \quad n=0,1,\ldots,N-1. \tag{39}$$

Then, if one uses the recurrence relation for the Chebyshev polynomial $T_k(x)$:

$$T_{k+1}(x) - 2xT_k(x) + T_{k-1}(x) = 0, \quad k=1,2,\ldots,$$

it is easy to see that $u_n(c)$ defined by (39) satisfies a three-term recurrence relation:

$$u_{n+1}(c) - 2cu_n(c) + u_{n-1}(c) = a_n^N - a_{n+2}^N, \quad n=N,N-1,\ldots,1, \tag{40}$$

where we define $a_{N+1}^N = a_{N+2}^N = 0$ and $u_N(c) = u_{N+1}(c) = 0$ for convenience.

From (38) it is seen that one can compute the first term in the right-hand side of (11) by the formula

$$2\sum_{n=0}^{[(N-1)/2]} \frac{u'_{2n}(c)}{2n+1}, \tag{41}$$

where $u'_n(c)$ denotes the derivative of $u_n(c)$ with respect to c. The recurrence (40) gives rise to the recurrence formula for $u'_n(c)$:

$$u'_{n+1}(c) - 2cu'_n(c) + u'_{n-1}(c) = 2u_n(c), \quad n=N,N-1,\ldots,1, \tag{42}$$

where we set $u'_N(c) = u'_{N+1}(c) = 0$ for convenience. It requires only $O(\frac{5}{2}N)$ multiplications (and divisions) to compute (41) for each c-value by using $u_n(c)$'s and $u'_n(c)$'s obtained from the backward recursions of (40) and (42), respectively.

Appendix B

Here we prove Lemma 3.3. If one notes that $T'_n(x) = nU_{n-1}(x)$, $n \geqslant 1$, and notes that $\int_{-1}^{1} T_n(x)\,\mathrm{d}x = 2/(1-n^2)$ if n is even, and vanishes otherwise, it follows from (25) that

$$\frac{\mathrm{d}S_m(x)}{\mathrm{d}x} = \sum_{n=0}^{M}{}' (m-2n)U_{m-2n-1}(x)\left(\frac{1}{2n+1} - \frac{1}{2n-1}\right), \quad m=1,2,\ldots, \tag{43}$$

where we set $M = [\frac{1}{2}(m-1)]$. It is easy to verify that $S'_1(x) = 1$, and that $|S'_2(x)| = 2|U_1(x)| \leqslant 4$, $-1 \leqslant x \leqslant 1$.

Using the identity $U_n(x) - U_{n-2}(x) = 2T_n(x)$, $n \geqslant 2$, in (43) yields

$$\frac{\mathrm{d}S_m(x)}{\mathrm{d}x} = 2\sum_{n=0}^{M-1} \frac{sT_{s-1}(x) + U_{s-3}(x)}{2n+1} + \frac{m-2M}{2M+1}U_{m-2M-1}(x), \tag{44}$$

where $s = m-2n$, $m=3,4,\ldots$.

Using in (44) the fact that $|T_n(x)| \leqslant 1$ and $|U_n(x)| \leqslant n+1$ gives the bound for $S_m'(x)$:

$$\left|\frac{\mathrm{d}S_m(x)}{\mathrm{d}x}\right| \leqslant 4m \sum_{n=0}^{M-1} \frac{1}{2n+1} + \frac{(m-2M)^2}{2M+1} - 4M, \quad m = 3, 4, \dots . \tag{45}$$

Lemma 3.3 follows easily, if one uses in (45) the relation

$$\sum_{n=0}^{K} \frac{1}{2n+1} \leqslant 1 + \tfrac{1}{2}\ln(2K+1), \quad K \geqslant 0.$$

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